1,1,1,3,3,3-Hexafluoropropan-2-yl trifluoroacetate
42031-15-2 | DTXSID80340673

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.39e-13 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 3.04e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

Image not found
Acetic acid, trifluoro-
Measured: 1.20e-13
Predicted: 1.81e-13

Image not found
1,1,2,3,3,3-Hexafluoro-1-propene
Measured: 2.20e-12
Predicted: 2.03e-12

Image not found
Trifluoro(trifluoromethoxy)ethylene
Measured: 3.58e-12
Predicted: 3.22e-12

Image not found
Acetic acid, trifluoro-, methyl ester
Measured: 5.20e-14
Predicted: 5.42e-14

Image not found
Hexafluorobenzene
Measured: 1.71e-13
Predicted: 6.65e-14